Application of COSMO-RS and UNIFAC for ionic liquids based gas separation

In recent years, due to their advantages on good stability, non-volatility, tunable viscosity and tailor-made properties, ionic liquids (ILs) have been regarded as novel potential solvents and alternative media for gas separation. However, the various cations and anions representing the ILs, together with limited experimental data, make it challenging to predict gas solubility in ILs and identify the optimal IL for a specific gas separation. In this work, a comprehensive Henry’s law constants database is first established for gas-IL which supplements an already established extensive gas solubility database. Because of the insufficient experimental data for both IL-C₂H₄ and IL-C₂H₆ systems, the COSMO-RS model is used after validation to generate additional pseudo-experimental data. Then, together with the sufficient experimental data of CO₂-IL and CH₄-IL systems, UNIFAC-IL is developed for the prediction of four-component shale gas (CH₄, C₂H₄, C₂H₆, CO₂) solubility in ILs. A relatively good agreement between the model predicted and the experimental solubility data is observed. Moreover, the developed UNIFAC-IL model can be used to predict the solubility of gases in new ILs that are not included in parameter fitting due to its group contribution basis. For this reason, the model represents a very useful tool for task-specific design of ionic liquids for gas separations.

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